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Electronic superstructures in doped semiconductor superlattices

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Abstract. We show that in doped semiconductor superlattices with narrow quantum wells at low temperatures and at sufficiently low doping levels, the exchange-correlation contribution to the system energy can exceed the sum of the kinetic and Hartree energies. Under these conditions, the uniform distribution of electrons over the wells becomes unstable, and the ground state corresponds to inhomogeneous distribution (electronic superstructure). For GaAs/GaAlAs superlattices the estimate of the critical doping concentration at which the stability of the homogeneous state at $T = 0$ K is lost yields the value of about 10^{17} cm^{-3}. Inhomogeneous ground states are discussed.

Introduction

The fact that the ground state of a system of interacting electrons can become inhomogeneous (Wigner crystallization [1]) has been widely discussed in the literature. However, the conditions for Wigner crystallization are very restrictive and, in the absence of magnetic field, it has only been observed in electron sheets over the surface of liquid helium. In semiconductor superlattices (SL), new possibilities for the formation of inhomogeneous states appear, in particular, related to inhomogeneous electron distribution over the wells of the SL. One of the mechanisms was discussed in [2], where the symmetry breaking resulted from the carrier delocalization in the second subband for some specific shapes of the SL profile. In [3], a different mechanism of symmetry breaking was suggested for doped SL with electrons in the lowest subband, related to the exchange-correlation contribution to the total energy of the system. In what follows, we present the analysis of the latter situation; we study the ground state at $T = 0$ K and the possibility of spontaneous symmetry breaking in a system of interacting electrons in doped compositional SL.

Density functional

It is convenient to use the approach based on the density functional theory. An important feature of the electron gas in a SL is that the confinement potential is generally not weak and forms the electronic states. We consider the case in which the wells of the SL are sufficiently narrow so that only the lowest subband is occupied, and moreover, the overlap of the wave functions of neighboring wells which determines the miniband width is sufficiently small. In this case one can use the method analogous to the tight binding approach and explicitly write the energy as the functional of the electron density n, thus making a straightforward analysis of the spatial distribution of the electron density possible. We have

$$E[n] = T[n] + E_{\text{Hartree}}[n] + E_{\text{ext}}[n] + E_{\text{xc}}[n], \tag{1}$$

where $T[n]$ is the kinetic energy of noninteracting electron gas, E_{Hartree} is the energy of electron-electron interaction calculated in the Hartree approximation (including the interaction with the positive background), E_{ext} is the energy of interaction with external fields (if present), and E_{xc} is the remaining part of the energy (the so called exchange-correlation energy). We write the functional (1) using the set of states in the confinement potential, so that the electron density is a function of $\{\rho, i\}$, where ρ is a radius vector in the well plane and i is the discreet well number.

In what follows we study distributions of electron density over the wells of the SL in the absence of external fields; we call a distribution inhomogeneous if it corresponds to different average in-plane concentrations for different wells. We shall see that the conditions for the transition to such inhomogeneous states are much less restrictive than conditions for Wigner crystallization for the two-dimensional electron gas in a well. For this reason, we can assume that the electron density is independent of ρ, $n = \sum_i \nu_i \delta(z - z_i)$, where z is the coordinate along the SL axis, $z_i = i\,d$, d is the SL period and ν_i is the two-dimensional density in the i th well; hence the density functional becomes simply a function of many variables $\nu = \{\nu_i\}$. For a small overlap, we can explicitly write the terms in the energy functional (1). The kinetic energy is additive,

$$T[\nu] = \sum_i T(\nu_i), \tag{2}$$

where $T(\nu_i) = 2\nu_i^2/2\rho_0$ is the kinetic energy of two-dimensional electron gas in the i th well and ρ_0 is the density of states in a well. For the Hartree contribution we have

$$E_{\text{Hartree}}[\nu] = \sum_{i,j} V_{ij}(\nu_i - \nu_0)(\nu_i - \nu_0), \tag{3}$$

where $V_{ij} = -(2\pi e^2 d/\epsilon)|i-j|$, ϵ is the dielectric constant, and ν_0 is the average electron concentration per well per unit area; for uniform donor doping $\nu_0 = N_d d$. For weak overlap of the wave functions of adjacent wells the exchange energy is also additive,

$$E_{\text{xc}}[\nu] = \sum_i E_{\text{xc}}(\nu_i), \tag{4}$$

where $E_{\text{xc}}(\nu_i) = C_{\text{xc}}(e^2/\epsilon)\nu_i^{3/2}$ is the exchange energy for two-dimensional electron gas in the i th well and $C_{\text{xc}} \approx 0.81$ [4, 5]. The correlation energy is additive, provided that the radius of the Coulomb hole is smaller than the distance between the wells, $\nu_0^{-1/2} << d$. At small concentrations, the additivity is no more valid; in this case, however, the correlation energy contribution plays minor role in the transition to inhomogeneous state, and for simplicity we restrict ourselves with the exchange contribution. It can be easily seen that the inclusion of correlation gives rise to a weakening (unessential for $\nu_0^{1/2} d << 1$) of the conditions for the transition to the inhomogeneous state.

Instability of the homogeneous distribution

Once the energy functional is explicitly known, we can study the stability of the homogeneous ground state with respect to small perturbations. It is known that both in three- and two-dimensional electron gas, the Wigner crystallization occurs via a spin-polarized

state [6, 7]. As follows from (1)–(4), the stability of the nonpolarized ground state in any of the layers with respect to transition to the spin-polarized state is lost if

$$\nu_0 < (3C_{xc}e^2\rho_0/2\epsilon)^2. \tag{5}$$

Taking account of the weak overlap of wave functions of adjacent wells, we can see that the lowest energy corresponds to the antiferromagnetic-type ordering of spin polarizations of adjacent layers.

The variation of (1)–(4) yields the following condition for the loss of stability of the spatially homogeneous state:

$$\frac{1}{\rho_0} + \frac{2\pi e^2 d}{\epsilon} - C_x \frac{3e^2}{4\epsilon\nu^{1/2}} < 0. \tag{6}$$

It is seen that condition (5) which determines the threshold impurity concentration N_d^* for the transition to the spin-polarized state is less strict than the condition for the loss of spatial homogeneity (6), i.e. the transition to an inhomogeneous state occurs via the spin-polarized state. This is due to the Hartee contribution which impedes the appearance of the inhomogeneous distribution. At the threshold concentration where the stability of the homogeneous solution is lost, the "most dangerous" density fluctuations are those corresponding to the period doubling. One can show that an inhomogeneous solution (electronic superstructure) with the period $2d$, stable with respect to small fluctuations, can exist for impurity concentrations $N_d < N_{d1}^*$, where $N_{d1}^* > N_d^*$. For $N_{d2}^* < N_d < N_{d1}^*$ it exists as a metastable state and then (for $N_d < N_{d2}^*$) it becomes the ground state. At still lower concentrations solutions with greater commesurate periods are also possible. It should be noted that the energy gain when an inhomogeneous state is formed decreases rapidly with decreasing concentration; accordingly, the temperature stability of the superstructures is expected to decrease at lower doping levels, and the intermediate concentrations are optimal for their observation.

Discussion

Thus in doped short-period doped SL, electronic superstructures (electron distributions over the wells inhomogeneous in the direction of the SL axis) can exist. The mechanism of spontaneous symmetry breaking in our case is, however, different from that of Wigner crystallization. Although formally the problem is reduced to a one-dimensional one, the transition is actually due to exchange interaction in quasi-two-dimensional quantum wells. The substantial weakening of the conditions for the transition to inhomogeneous ground state is due to the following reasons. In the theory of Wigner crystallization, the local density approximation in the density functional theory is known to appreciably overestimate the threshold concentrations, as is seen, e.g., from Monte Carlo calculations [7, 8]. This reflects the important role of corrections in the gradient expansion of the density functional. In our case, the overlap integral plays the role similar to that of gradient corrections, the expression for the density functional is similar to that of the local density approximation and the role of overlap corrections is actually small.

One can estimate the concentration of the doping impurity corresponding to the creation of the superstructure at $T = 0$ K. Taking $\rho_0 = 3 \cdot 10^{13}$ eV^{-2} cm^{-2}, $\epsilon = 12.7$, and $d = 9$ nm, we obtain for the critical donor concentration $N_{d2}^* \approx 8 \cdot 10^{16}$ cm^{-3}. This indicates the possibility of the existence of electronic superstructures in doped SL under

conditions essentially less restrictive than those for the Wigner crystal. The appearance of the superstructure is expected to have much more pronounced effect on vertical transport in SL than the transition to the spin-polarized state. In fact, it is accompanied by the shifts of the size quantization levels in adjacent wells and by the appearance the gap in the spectrum of elementary excitations related to charge transfer between the wells. These excitations actually determine the vertical (in the direction of the SL axis) conductivity of the structure at finite temperatures. Vertical conductivity anomalies observed in doped GaAs/GaAlAs SL [3] just at impurity concentration 10^{17} cm^{-3} might be related to the emergence of the superstructure.

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